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Supporting Information for Szyperski et al. (2002) Proc. Natl. Acad. Sci. USA 99 (12), 8009–8014. (10.1073/pnas.122224599).

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Supporting Figure 12

Fig. 12. Experimental scheme for the 2D 1 H-TOCSY-relayed-<u>HC</u>H-COSY experiment. Rectangular 90° and 180° pulses are indicated by thin and thick vertical bars, respectively, and phases are indicated above the pulses. Where no rf phase is marked, the pulse is applied along x. The high-power 90° pulse lengths were: 5.9 ms for 1 H and 15.4 ms for 13 C. The 1 H rf carrier is placed at the position of the solvent line at 4.78 ppm, and the 13 C carrier is set to 131 ppm. GARP is used for 13 C decoupling during acquisition (rf field strength = 2.5 kHz), and 1 H isotropic mixing is accomplished using the DIPSI-2 scheme (rf = 16 kHz). The duration and strengths of the pulsed z-field gradients (PFGs) are: G1 (1 ms, -10 G/cm); G2 (500 ms, 6 G/cm); G3 (500 ms, 7.5 G/cm); G4 (1 ms, 22 G/cm). All PFG pulses are of rectangular shape. A recovery delay of at least 100 ms duration is inserted between a PFG pulse and an rf pulse. Water suppression is accomplished by presaturation of the water line during the relaxation delay. The delays are: $t_1 = 3.0$ ms, $t_2 = 15.38$ ms. Phase cycling: $f_1 = x$, -x, $f_2 = x$, x, y, y, -x, -x, -y, -y, $f_3 = 4(x)$, 4(y), 4(-x), 4(-y); $f_4 = x$, x, -x, -x

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